

# Discrete quantum square well of the first kind.

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## Abstract

A new exactly solvable cryptohermitian quantum chain model is proposed and analyzed. Its discrete-square-well-like Hamiltonian with the real spectrum possesses a manifestly non-Hermitian form. It is only made self-adjoint by the constructive transition to an *ad hoc* Hilbert space. Such a space (i.e., the closed form of its inner product, i.e., the “metric”  $\Theta$ ) varies with an  $N$ -plet of optional parameters. The simplicity of our model enables one to obtain the complete family of these physics-determining metrics  $\Theta$  in a user-friendly band-matrix closed form.

## 1 Introduction

One of the most remarkable features of quantum mechanics may be seen in the robust nature of its “first principles” and probabilistic interpretation. These principles practically did not change during the last cca eighty years. In a sharp contrast, the production of the innovative applications of the theory does not seem to have ever slowed down.

In particular, twenty years ago, Scholtz et al [1] emphasized that the *dynamical* content of the phenomenological models of microscopic systems may be encoded not only in the Hamiltonians and other observables but also, equally efficiently, in metric operators  $\Theta$  defining certain nontrivial, “sophisticated” representations  $\mathcal{H}^{(S)}$  of the physical Hilbert space of the bound states of the quantum system in question<sup>1</sup>.

It is worth noticing that in *loc. cit.* the authors had in mind, first of all, the physical systems as “traditional” as the heavy atomic nuclei. During the recent renaissance of the theory the use and appeal of nontrivial metrics  $\Theta^{(S)} \neq I$  has significantly been extended. In particular, the recent reviews [3, 4, 5] of the so called  $\mathcal{PT}$ -symmetric quantum mechanics may be recalled as describing, in detail, a number of the less traditional explicit models, with the applicability ranging from the very pragmatic phenomenological fits of spectra up to the ambitious theoretical proposals throwing new light

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<sup>1</sup>in *loc. cit.* the authors decided to denote the Hilbert-space metric by the symbol  $T$ ; we shall prefer the use of the “Greek translation” of this letter - see also [2] for explanation

on various old questions (the most recent proceedings [6] may be also recalled as a recommended introductory reading).

In the particular  $\mathcal{PT}$ -symmetric theoretical framework one selects just a very specific subclass of eligible metrics  $\Theta_{\mathcal{PT}}^{(S)}$  which prove expressible as products of parity  $\mathcal{P}$  and charge  $\mathcal{C}$ . In practice, unfortunately, the simplicity of such a recipe appeared to be accompanied by its conceptual weakness and non-applicability in the scattering regime [7]. This strongly motivated a subsequent return to the study of the other models characterized by the potentially broader variability of the Hilbert-space metric [8, 9].

Unfortunately, the latter return to the less straightforward model-building recipes has been accompanied by the perceivable growth of technical difficulties [10]. For this reason, the attention of many authors has been re-attracted to the quantum models in which the use of a nontrivial metric  $\Theta^{(S)} \neq \Theta_{\mathcal{PT}}^{(S)}$  gets combined with very schematic and “user-friendly” Hamiltonians  $H$ . *Pars pro toto* let us recollect one of the most elementary illustrative examples provided by the square-well Hamiltonian  $H$  of Ref. [11] accompanied by the nontrivial metrics  $\Theta^{(S)}$  proposed by Mostafazadeh and Batal [12].

The latter authors emphasized that the physical content of the quantum models described by the *pairs* of the operators  $(H, \Theta)$  remains entirely standard and compatible not only with the very general recipe and formalism of Ref. [1] but also, at least implicitly, with any current textbook on quantum mechanics. In particular, the authors constructed the related position and momentum operators and explained the existence of the conserved probability density as well as the feasibility of the more or less standard backward transition to the classical, non-quantum limit.

In what follows we intend to describe a new square-well-related quantum model. Although we shall mainly pay attention to its formal aspects, physics-motivated readers may equally well reveal a strong phenomenological appeal of our present model in its very close formal as well as qualitative link to the above-mentioned square-well system. Moreover, in the light of the recent literature the independent and purely experimental appeal of the similar models has recently been found even in *non-quantum* physics [13].

Our message will be organized as follows. In section 2 we shall review a few older relevant results. Subsequently, in section 3 we shall restrict our attention to the new, extremely elementary Chebyshev-lattice Hamiltonian. We shall describe the properties of this quantum model in detail. In section 4 we shall finally pay attention to the parametric-dependence of the associated “sophisticated” physical Hilbert space(s).

All of these results will indicate that even when the Hamiltonian matrix itself remains comparatively elementary, the quantum dynamics of the system may remain rich in a way mediated by the variability of the “sophisticated” physical Hilbert space. The existence of certain Hilbert-space-induced boundaries of the observability of the quantum system in question will be pointed out. Their shape will be shown to vary with our choice of the optional parameters determining the (ambiguous) Hilbert space. This and other observations will be explained and summarized in section 5.

## 2 Framework: Quantum chain models

### 2.1 Discrete quantum square wells

It is well known [14] that the discrete square-well Schrödinger equation

$$H^{[U]} |\psi_n^{[U]}\rangle = E_n^{[U]} |\psi_n^{[U]}\rangle, \quad n = 0, 1, \dots, N-1 \quad (1)$$

with the real,  $N$  by  $N$  Hamiltonian matrix

$$H^{[U]} = \begin{bmatrix} 0 & 1 & 0 & \dots & 0 \\ 1 & 0 & 1 & \ddots & \vdots \\ 0 & 1 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 0 & 1 \\ 0 & \dots & 0 & 1 & 0 \end{bmatrix} \quad (2)$$

is exactly solvable in terms of the Chebyshev's polynomials of the second kind<sup>2</sup>,

$$|\psi_n^{[U]}\rangle = \begin{bmatrix} U(0, x_n) \\ U(1, x_n) \\ \vdots \\ U(N-1, x_n) \end{bmatrix}. \quad (3)$$

On this background, let us call this model, for our present purposes, the discrete quantum square well of the second kind. For this model it is worth noticing that the related bound-state spectrum of energies  $E_n^{[U]} = 2x_n$  is all available in closed form,

$$E_n^{[U]} = 2 \cos \frac{(n+1)\pi}{N+1}, \quad n = 0, 1, \dots, N-1. \quad (4)$$

This “square-well model of the second kind” can immediately be identified with the discrete version of the standard Schrödinger's differential-equation square-well problem [17]. Hence, its large- $N$  limit remains well understood and solvable.

In our present letter we intend to introduce a similar “square-well model of the first kind” obtained via a replacement of the elements of the quantum state vectors (3) by the equally friendly Chebyshev polynomials of the first kind,

$$|\psi_n^{[T]}\rangle = \begin{bmatrix} T(0, x_n) \\ T(1, x_n) \\ \vdots \\ T(N-1, x_n) \end{bmatrix}. \quad (5)$$

It is easy to show that with  $E_n^{[T]} = 2x_n$  such an ansatz will be compatible with the alternative square-well-type Schrödinger equation

$$H^{[T]} |\psi_n^{[T]}\rangle = E_n^{[T]} |\psi_n^{[T]}\rangle, \quad n = 0, 1, \dots, N-1 \quad (6)$$

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<sup>2</sup>our denotation of these polynomials is borrowed from MAPLE [15]; for our present purposes it proves much better suited than their more common subscripted symbols [16].

in which another real though manifestly non-Hermitian Hamiltonian-type matrix is being used,

$$H^{[T]} = \begin{bmatrix} 0 & 2 & 0 & \dots & 0 \\ 1 & 0 & 1 & \ddots & \vdots \\ 0 & 1 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 0 & 1 \\ 0 & \dots & 0 & 1 & 0 \end{bmatrix}. \quad (7)$$

Although the latter Hamiltonian matrix only marginally (i.e., in the single matrix element) differs from its square-well predecessor (2), both of these models lead to the perceivably different (though, in both cases, robustly real) spectra of energies, with Eq. (4) complemented by the equally elementary formula

$$E_n^{[T]} = 2 \cos \frac{(n + 1/2)\pi}{N}, \quad n = 0, 1, \dots, N - 1, \quad (8)$$

This conclusion may easily be verified by the insertion of the  $N$ -dimensional ket-vector ansatz (5) into our Schrödinger Eq. (6) + (7).

One reveals that our two models share the same formal merit of having their energies  $E_n = 2x_n$  given in terms of the roots of the very similar respective secular equations  $U(N, x_n) = 0$  and  $T(N, x_n) = 0$ . Naturally, the manifestly non-symmetric (i.e., non-Hermitian) form of the latter Hamiltonian (7) violates the analogy and requires an appropriate amendment of the underlying physical Hilbert space of states (cf. our recent review [2] as summarized in Appendix A below). In our present letter we simply intend to discuss and remove the latter, purely technical obstacle.

## 2.2 The trick of the Hermitization

Among applications of quantum theory there exists a striking contrast between the widely employed variability and adaptability of Hamiltonians  $H$  (which, by construction, have to generate the unitary time evolution) and a very rare use of the equally admissible variability of the eligible (i.e., symbolically,  $\kappa$ -numbered or  $\vec{\kappa}$ -numbered) alternative representations of the Hilbert space  $\mathcal{H} = \mathcal{H}(\vec{\kappa}_0)$  of admissible states.

In our research we felt addressed by this disproportion. Naturally, we understood that the widespread practice of choosing, predominantly, just the “most friendly” Hilbert-space representation  $\mathcal{H}^{(F)} = L^2(\mathbb{R})$  (and/or its inessential modifications) is only based on certain extremely formal grounds (cf. the critique of this purely comfort-based habit, say, in [3]).

In the notation summarized briefly in Appendix A below let us consider, therefore, the less conventional and less restrictive approach to quantum model-building in which a given quantum system is described not only by its Hamiltonian  $H$  (which will be, generically, non-Hermitian in the randomly selected “first-option” Hilbert space  $\mathcal{H}^{(F)}$ ) but also by the related (and, generically, necessarily nontrivial) suitable metric operator  $\Theta \neq I$ .

In this context our present paper intends to offer a sufficiently transparent illustration of the feasibility of working with variable multiindices  $\vec{\kappa}$  in the operator doublets  $(H, \Theta(\vec{\kappa}))$ . For this purpose we shall accept a few drastic simplifications of the technicalities, assuming that

- both  $H$  and  $\Theta$  are just the real,  $N$  by  $N$ -dimensional matrices with an arbitrary finite (though freely variable) dimension  $N = 1, 2, \dots$ ;
- the “well-studied” consequences of the possible variations of  $H$  will be ignored and suppressed; just the single sample of  $H$  will be considered.

We shall mainly be interested in the physics-influencing consequences of the variability of  $\Theta = \Theta(\vec{\kappa})$ . Once we intend to study just nontrivial metrics, the Hamiltonian matrix itself will be required non-Hermitian in the trivial (and, hence, unphysical) Hilbert space  $\mathcal{H}^{(F)}$ ,  $H \neq H^\dagger$ .

### 2.3 The nearest-neighbor-interaction lattices

Among all of the finite-dimensional Schrödinger equations

$$\hat{H} |\psi_n^{(N)}\rangle = E_n^{(N)} |\psi_n^{(N)}\rangle, \quad n = 0, 1, \dots, N-1 \quad (9)$$

with the  $N$  by  $N$  Hamiltonian matrices  $\hat{H}$  possessing real spectra  $\{E_n^{(N)}\}$  a privileged, most efficiently solvable subclass is formed by the “chain” models in which the matrix  $H$  is tridagonal,

$$\hat{H} = \begin{bmatrix} a_1 & c_1 & 0 & 0 & \dots & 0 \\ b_2 & a_2 & c_2 & 0 & \dots & 0 \\ 0 & b_3 & a_3 & c_3 & \ddots & \vdots \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & b_{N-1} & a_{N-1} & c_{N-1} \\ 0 & \dots & 0 & 0 & b_N & a_N \end{bmatrix}. \quad (10)$$

Often, these models are studied as mimicking an  $N$ -site quantum-lattice dynamics containing just the nearest-neighbor interaction (cf., e.g., [18]).

A simplification of the model may be achieved when our Schrödinger Eq. (9) + (10) becomes solvable in closed form. Two illustrations of the specific merits of such an approach may be found in our recent papers [19, 20]. We studied there the exactly solvable models in which the *explicit* form of the eigenvectors  $|\psi_n^{(N)}\rangle$  was obtained in the following two alternative forms defined either in terms of the Gegenbauer classical orthogonal polynomials  $G(n, a, x)$ ,

$$|\psi_n^{(N)}\rangle \equiv |\psi_n^{[G]}(a)\rangle = \begin{bmatrix} G(0, a, E_n) \\ G(1, a, E_n) \\ \vdots \\ G(N-1, a, E_n) \end{bmatrix} \quad (11)$$

or in terms of the Laguerre polynomials  $L(n, a, x)$ ,

$$|\psi_n^{(N)}\rangle \equiv |\psi_n^{[L]}(a)\rangle = \begin{bmatrix} L(0, a, E_n) \\ L(1, a, E_n) \\ \vdots \\ L(N-1, a, E_n) \end{bmatrix}. \quad (12)$$

Due to the necessity of having a Hamiltonian with a free parameter  $\lambda \equiv a$  at our disposal, we had to accept the serious shortcoming of both of these models, viz, the purely numerical character of the determination of the respective energies  $E_n^{(N)} \equiv E_n^{[G]}(a)$  and  $E_n^{(N)} \equiv E_n^{[L]}(a)$  at the general dimension  $N$ .

In this context our present paper has been motivated by the intention to simplify the calculations and, in particular, to get rid of the necessity of the numerical determination of the energies.

### 3 The variability of the metric for $H = H^{[T]}$

Recalling the experience gained within the  $\mathcal{PT}$ -symmetric quantum mechanics one may employ a “sophisticated” physical Hilbert space with non-trivial metric, viz.,  $\mathcal{H}^{(S)} \neq \mathcal{H}^{(F)}$ . Then, the Hermiticity of the matrix  $H$  in simple-minded space  $\mathcal{H}^{(F)}$  need not be considered obligatory [3]. In this setting our present paper may be perceived as inspired by Refs. [19, 20], i.e., by the feasibility of the construction of the solvable chain models of the form (11) and (12). The non-numerical nature of the related constructions of the metrics enabled us to obtain the fairly large, multi-labeled set of the user-friendly “Hermitization” recipes which varied with a multiindex  $\vec{\kappa}$  in metrics  $\Theta = \Theta(\vec{\kappa})$ .

In a short detour let us mention that the multiindex-controlled variability of the metrics has been first considered useful in nuclear physics [1]. The implementation of the fully general description of a quantum system by means of the preselected pair of operators  $H(\lambda)$  and  $\Theta(\kappa)$  has been recommended there as a direct tool of the construction of phenomenological models. The different choices of the metric have been identified there with the alternative specifications of the different admissible sets of operators of observables. In this sense, the generic change of multiindex  $\lambda$  or  $\kappa$  plays the same dynamical role of the control of measurable predictions.

The domain  $\mathcal{D}^{(H)}$  of the variability of the Hamiltonian-controlling or “coupling” parameters  $\lambda$  themselves would be bounded by the points at which the spectrum of  $H(\lambda)$  (i.e., of energies of the system) ceases to be real and, hence, observable. These points of boundary  $\partial\mathcal{D}^{(H)}$  are called exceptional points. Many years ago their exact definition has been given by Kato [21]. At present, their phenomenological role is being intensively studied [22].

The physical interpretation as well as the boundaries of admissibility specify the second parametric domain  $\mathcal{D}^{(\Theta)}$  of the physics-compatible set of parameters  $\kappa$  (entering the metric) in a less straightforward manner. This inspired our present study. We shall select a parameter-free Hamiltonian  $H$  and vary just the metrics  $\Theta = \Theta(\kappa)$ . In this manner we shall be able to study the mechanisms by which the concept of the horizon of the observability of the underlying quantum system is put into a Hamiltonian-independent perspective.

#### 3.1 The closed formula for the metrics $\Theta = \Theta^{[T]}(\vec{\kappa})$ .

Given the two alternative initial  $N$  by  $N$  tridiagonal real matrices (2) and (7) one would have a tendency of skipping, as unphysical, the latter possibility with non-Hermitian Hamiltonian  $H^{[T]} \neq (H^{[T]})^\dagger$ . In the spirit of the

conventional textbooks only the former option with  $H^{[U]} = (H^{[U]})^\dagger$  would survive. In our present, methodically oriented paper we shall follow the guidance given by Refs. [19, 20] which allows us to ignore, on the contrary, the former Hermitian Hamiltonian  $H^{[U]}$  as not too interesting.

Under the assumption  $H \neq H^\dagger$ , naturally [23], one has to replace the single Schrödinger Eq. (9) by the doublet of the left-eigenvector and right-eigenvector problems. Using our notation of review paper [2] with doubly-marked left eigenvectors this pair of equations reads

$$H |\psi_n\rangle = E_n |\psi_n\rangle, \quad \langle\langle \psi_n | H = E_n \langle\langle \psi_n | \quad (13)$$

or, equivalently,

$$H |\psi_n\rangle = E_n |\psi_n\rangle, \quad H^\dagger |\psi_n\rangle\rangle = E_n^* |\psi_n\rangle\rangle. \quad (14)$$

Under the assumption that the spectrum is real and non-degenerate it is easy to recall the standard rules of linear algebra and to deduce that the resulting two  $N$ -plets of eigenvectors form a bicomplete biorthogonal basis,

$$I = \sum_{n=0}^{N-1} |\psi_n\rangle \frac{1}{\langle\langle \psi_n | \psi_n \rangle} \langle\langle \psi_n |, \quad \langle\langle \psi_m | \psi_n \rangle = \delta_{m,n} \langle\langle \psi_n | \psi_n \rangle. \quad (15)$$

In Ref. [24] we explained that such a separation of the kets from the ketkets implies that the Mostafazadeh's [23] general definition of the metric may be written in the spectral-representation form

$$\Theta = \sum_{n=0}^{N-1} |\psi_n\rangle\rangle |\nu_n|^2 \langle\langle \psi_n | \quad (16)$$

where the  $N$ -plet of complex parameters  $\nu_n \neq 0$  is arbitrary.

### 3.2 The simplified metrics and pseudometrics

For our present concrete toy-model Hamiltonian (7) the known form (5) of the quantum-lattice-site ket-components  $\{\alpha|\psi^{[T]}\rangle$  with  $\alpha = 1, 2, \dots, N$ , i.e., formulae

$$\begin{aligned} \{1|\psi^{[T]}\rangle &= T(0, x) = 1, & \{2|\psi^{[T]}\rangle &= T(1, x) = x, \\ \{3|\psi^{[T]}\rangle &= T(2, x) = 2x^2 - 1, & \dots, & \{N|\psi^{[T]}\rangle = T(N-1, x) \end{aligned} \quad (17)$$

may be complemented, after some algebra, by their ketket-component counterparts

$$\{1|\psi^{[T]}\rangle\rangle = T(0, x)/2 = 1/2, \quad \{\alpha|\psi^{[T]}\rangle\rangle = T(n, x), \quad \alpha = 2, 3, \dots, N. \quad (18)$$

This means that the difference between these two sets only emerges at the single site-index  $\alpha = 1$ . As the main consequence of such a not entirely expected simplicity of the left eigenvectors (18), the above-mentioned general  $N$ -term spectral-expansion sum (16) + (18) may be reclassified, for our  $H = H^{[T]}$ , as a very rare closed-form definition of the complete set of the matrices of the eligible metrics.

Naturally, the latter formula covers all of the possible special cases and choices of the optional  $n$ -plets of parameters  $\nu_n \neq 0$ . In this sense its practical usefulness is universal. Still, the resulting generic form of the metric is a general matrix containing as many as  $N$  free parameters  $|\nu_n|^2 > 0$ . Fortunately, in the light of the experience gained in Refs. [19, 20] one can expect that such a complete set of the eligible metrics can be split into subsets of certain much simpler, sparse-matrix form.

The same possibility also emerges in our present Chebyshevian quantum lattice. The sparsity of the metrics may be achieved when one replaces the fully general recipe (16) + (18) by its implicit, linear-algebraic-equation version in which a suitable ansatz for  $\Theta$  is inserted in matrix equation

$$H^\dagger \Theta = \Theta H. \quad (19)$$

Surprisingly enough, such an approach will enable us to make full use of the chain-model tridiagonality (10) of  $H$  and to complement it by the tentative parallel assumption of the band-matrix form of the metrics.

Once this idea is implemented, one immediately arrives at the simplest possible (and, up to an irrelevant overall factor, parameter-independent) form of the diagonal-metric solution of Eq. (19),

$$\Theta_{\alpha,\beta}^{(diagonal)} = \delta_{\alpha,\beta}(1 - \delta_{\alpha,1}/2) \Theta_{N,N}^{(diagonal)}, \quad \alpha, \beta = 1, 2, \dots, N. \quad (20)$$

By the similar technique, the next, one-parametric tridiagonal candidate for the metric is found to have the universal  $N$ -dimensional matrix form

$$\Theta^{(N)}(\lambda) = \begin{bmatrix} 1/2 & \lambda & 0 & 0 & \dots & 0 \\ \lambda & 1 & \lambda & 0 & \ddots & \vdots \\ 0 & \lambda & 1 & \ddots & \ddots & 0 \\ 0 & 0 & \ddots & \ddots & \lambda & 0 \\ \vdots & \ddots & \ddots & \lambda & 1 & \lambda \\ 0 & \dots & 0 & 0 & \lambda & 1 \end{bmatrix}. \quad (21)$$

Next, the pentadiagonal, two-parametric formula is obtained,

$$\Theta^{(N)}(\lambda, \mu) = \left[ \begin{array}{cc|ccc|c} 1/2 & \lambda & \mu & 0 & \dots & 0 & 0 \\ \lambda & 1 + \mu & \lambda & \mu & 0 & \dots & 0 \\ \hline \mu & \lambda & 1 & \lambda & \mu & \ddots & \vdots \\ 0 & \mu & \lambda & 1 & \ddots & \ddots & 0 \\ 0 & 0 & \mu & \ddots & \ddots & \lambda & \mu \\ \vdots & \vdots & \ddots & \ddots & \lambda & 1 & \lambda \\ \hline 0 & 0 & \dots & 0 & \mu & \lambda & 1 - \mu \end{array} \right], \quad (22)$$

with the only irregularities at the triplet of diagonal elements  $\Theta_{j,k}^{(N)}(\lambda, \mu)$  with  $(j, k) = (1, 1), (2, 2)$  and  $(N, N)$ . Etc.

## 4 The positivity of the metrics

By the universal, non-sparse-matrix formula (16) the necessary condition of the positivity of the metric is trivially satisfied. Once we restrict our



attention to the sparse-matrix metrics, the problem of the guarantee of the positivity of the solution  $\Theta$  of Eq. (19) reemerges and has to be treated, e.g., perturbatively [20]. For our present, extremely simple toy model  $H^{[T]}$ , a few much stronger results (or at least conjectures) can be found and formulated, indeed.

#### 4.1 The eigenvalues of matrices $\Theta(\vec{\kappa})$

The price to be paid for the sparsity of the illustrative matrices (21) and (22) (which were obtained via an appropriate ansatz and direct brute-force solution of the set of  $N^2$  linear algebraic Eqs. (19)) lies in the loss of connection with Eq. (16), i.e., in the loss of the direct control of the necessary positivity of *all* of the free parameters  $|\nu_n|^2$ . Fortunately, such a shortcoming may be perceived as more than compensated not only by the almost complete survival of the mathematical simplicity of the formulae for the inner products based on nontrivial  $\Theta \neq I$  (cf. Appendix A) but, first of all, by the parallel partial preservation of the physical concept of the (possibly, “smeared” [20]) locality of the interaction (cf. also a few comments in Refs. [7] and [25] in this respect).

In opposite direction, it is easily verified by immediate insertions that the direct use of formula (16) + (18) always determines just the generic metric in its generic form of a full, “long-ranged” matrix. This is the “worst possible” scenario, from the point of physics at least. Indeed, in such a case our initial, intuitive but rather natural “nearest-neighbor-interaction” interpretation of Hamiltonians (10) is lost.

A reasonable (i.e., recommended) compromise may be seen in the use of the few-parametric and band-matrix forms of the metrics which remain easily obtainable and which are sampled by Eqs. (21) and (22). This class of solutions of Eq. (19) may be perceived as mathematically exceptional as well as intuitively appealing. In phenomenological context, they will certainly facilitate any physics-determining specification of the metric-compatible forms of all of the eligible operators representing, in principle, the observable quantities [1].

A more quantitative argument which might support the preference of the band-matrix metrics  $\Theta(\vec{\kappa})$  emerged during the purely numerical study of certain cryptohermitian discrete quantum graphs [26]. Empirically we found out, typically, that the volume of the domain of the positivity of the metrics (to be denoted here by the symbol  $\mathcal{D}^{(\Theta)}$ ) did not get too small when one restricted attention just to a sparse, band-matrix form of the metric.

#### 4.2 The horizons of the observability $\partial\mathcal{D}^{(\Theta)}$ at $N = 6$

In Eq. (21) and the like we need not necessarily be willing or able to guarantee that the parameter  $\lambda$  lies in the corresponding physical domain  $\mathcal{D}^{(\Theta)}$ . In such a case we shall sometimes denote the matrix  $\Theta^{(N)}(\lambda)$  by the symbol  $K^{(N)}(\lambda)$  (in tridiagonal case) or  $L^{(N)}(\lambda)$  (in pentadiagonal case) etc. Such matrices may still play the role of Krein-space or Pontryagin-space pseudometrics, provided only that none of their eigenvalues vanishes [27].

The first graphical guide to the discussion of these characteristics of the formal solution  $K^{(N)}(\lambda)$  of Eq. (19) is provided, at  $N = 6$ , by Fig. 1 where

all of the six eigenvalues  $k_j$  of  $K^{(N)}(\lambda)$  are displayed as functions of an unrestrictedly varied optional parameter  $\lambda$ . This illustrative graph might be replaced by the easy rigorous proofs (left to the readers) that

(1) matrix  $K^{(6)}(\lambda)$  defines the (positive definite) metric  $\Theta^{(6)}(\lambda)$  if and only if  $|\lambda| < 0.5176380902 = 2\lambda_{min}^{(6)}$  where  $\lambda_{min}^{(6)} = 0.2588190451$  is the smallest positive zero of  $T(6, \lambda)$ ;

(2) matrix  $K^{(6)}(\lambda)$  specifies the parity-resembling pseudometric  $\mathcal{P}^{(6)}(\lambda)$  (with the three positive and three negative eigenvalues) if and only if  $|\lambda| > 1.931851653 = 2\lambda_{max}^{(6)}$  where  $\lambda_{max}^{(6)} = 0.9659258265$  is the largest zero of  $T(6, \lambda)$ ;

(3) finally, matrix  $K^{(6)}(\lambda)$  possesses strictly one negative eigenvalue for  $2\lambda_{min}^{(6)} < |\lambda| < \lambda_{med}^{(6)}$  where  $\lambda_{med}^{(6)} = 0.7071067812$  is the remaining, third positive zero of  $T(6, \lambda)$ .

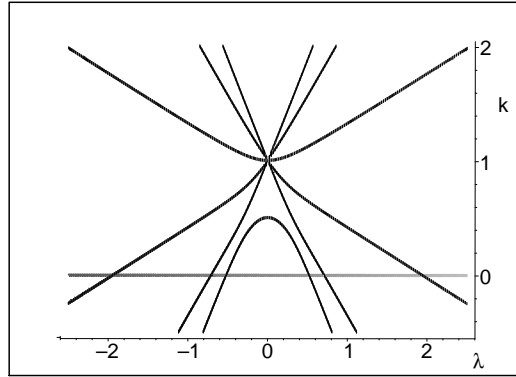


Figure 1: The  $\lambda$ -dependence of the sextuplet of the eigenvalues of matrix  $K^{(6)}(\lambda)$  of Eq. (21).

At the sufficiently small real values of parameter  $\lambda$  our matrices  $K^{(N)}(\lambda)$  remain positive definite, i.e., eligible as the desired and necessary metrics at any  $N$ . All of them define the corresponding particular admissible physical Hilbert space.

At  $N = 6$  it is still easy to move beyond the perturbation regime. It is possible to prove that up to the single remote and weakly  $\lambda$ -dependent lowest eigenvalue  $k_1(\lambda) \sim 1/2$  of  $K^{(6)}(\lambda)$ , the remaining quintuplet forms a locally linear left-right symmetric star with the center at the quintuply degenerate eigenvalue 1 at  $\lambda = 0$ . Thus, we may set  $k_j(\lambda) = 1 + \lambda y(\lambda)$  yielding the simplified secular equation

$$-2\lambda^5 y^3 - 5\lambda^6 y^4 + 3/2\lambda^5 y + 6\lambda^6 y^2 + 1/2 y^5 \lambda^5 + y^6 \lambda^6 - \lambda^6 = 0.$$

Once we factor out  $\lambda^5$  we obtain the five leading-order solutions  $y_0(\lambda) \rightarrow 0$  and  $y_{\pm 1}^2(\lambda) \rightarrow 1$  or  $y_{\pm 2}^2(\lambda) \rightarrow 3$  in the limit  $\lambda \rightarrow 0$ .

Another star-shaped dependence of the same eigenvalues emerges at the large  $|\lambda| \gg 1$ , i.e., asymptotically. At the even  $N = 2p$  we get strictly  $p$  linear asymptotes moving up and strictly  $p$  asymptotes moving down with the growth of  $|\lambda|$ , i.e., a Krein-space-pseudometric scenario.

At  $p = 3$  it is still easy to show, non-numerically, that one gets the sextuplet of asymptotic coefficients  $y \approx \pm 1.246979604, \pm 0.4450418679$  and  $\pm 1.801937736$  which, incidentally, coincide with the six roots of  $U(6, y)$ . Also a generalization of this observation to all  $p$  would be straightforward.

On this basis one may arrive at a remarkable conclusion that the variation of  $\lambda$  in our matrix  $K^{(6)}(\lambda)$  in fact interpolates between the interval of small  $\lambda$  (in which  $K^{(6)}(\lambda)$  may be treated as a metric in an appropriate Hilbert space) *and* the domain of very large  $\lambda$  (in which the same matrix  $K^{(6)}(\lambda)$  acquires the meaning of the metric in Krein space).

### 4.3 The horizons of the observability $\partial\mathcal{D}^{(\Theta)}$ at the larger even $N = 2p$

For the sake of brevity let us now skip the cases with the odd dimensions  $N$ . Then, taking any even  $N = 2p$  one specifies, in the similar manner as above, the domain  $\mathcal{D}^{(\Theta)}$  of the parameters guaranteeing the positivity of the tridiagonal band-matrix candidate (21) for the metric  $\Theta$ . The changes of the overall pattern of this construction with  $N$  are inessential. In particular, the above picture may be paralleled by its  $N = 8$  descendant displayed in Fig. 2.

One can summarize that in the tridiagonal case the single-parametric candidates  $\Theta(\lambda)$  become tractable as the true and positive matrices of the metric, provided only that the selected value of  $\lambda$  lies inside the well defined and  $N$ -dependent interval  $\mathcal{D}^{(\Theta)}$ . It's boundary points may be shown to be defined as the, in absolute value, smallest roots of  $U(2p, \lambda)$ , i.e.,

$$\lambda \in \mathcal{D}^{(\Theta)} = \left( \cos \frac{(p+1)\pi}{2p+1}, \cos \frac{(p)\pi}{2p+1} \right), \quad N = 2p. \quad (23)$$

From the phenomenological point of view these boundary points may be perceived as certain “horizons” of the observability of the system in question (cf. [2] for more details).

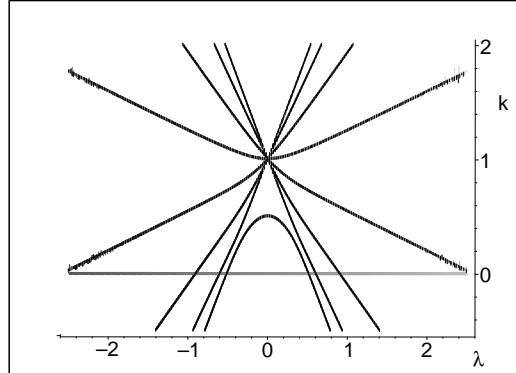


Figure 2: The  $\lambda$ -dependence of the eigenvalues of matrix  $K^{(N)}(\lambda)$  of Eq. (21) at  $N = 8$ .

### 4.4 The case of pentadiagonal metrics

Once we replace the above mentioned tridiagonal ansatz for  $\Theta$  by its next, pentadiagonal analogue, you may insert this ansatz in Eq. (19) and deduce the general form (22) of the candidate matrix  $L^{(8)}(\lambda, \mu)$ . Once we set here  $\lambda = 0$  we may study the differences from the previous case by its comparison with Fig. 3.

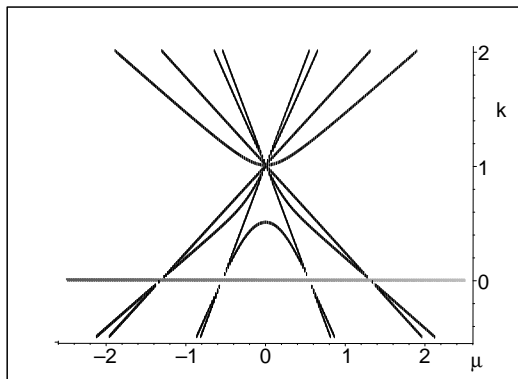


Figure 3: The  $\mu$ -dependence of the  $\lambda = 0$  eigenvalues of matrix  $L^{(8)}(\lambda, \mu)$ .

A new phenomenon emerges in the form of the degeneracy of vanishing eigenvalues. In Fig. 3 this may be seen as occurring at  $\lambda = 0$  and at  $\mu = \sqrt{1 \pm \sqrt{1/2}} = 0.5411961001, 1.306562965$ .

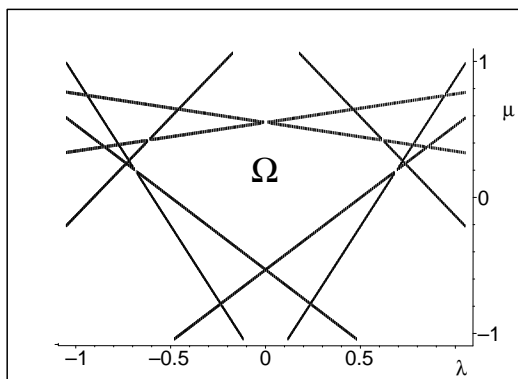


Figure 4: The domain  $\Omega$  of positivity of matrix  $L^{(8)}(\lambda, \mu)$ .

Our last, less restricted and fully two-parametric illustrative sample of the boundaries of the physical domain for the candidate matrix  $L^{(8)}(\lambda, \mu)$  is provided by Fig. 4. We see there that the boundaries (i.e., physical horizons) are formed by the straight lines. This just reflects the unexpected, difficult-to-reveal and difficult-to-prove observation (and, perhaps, an  $N$ -independent conjecture) that the corresponding polynomial in two variables which defines the physical horizon  $\partial\mathcal{D}^{(\Theta)}$  happens to be, in our particular model, completely factorizable over reals.

## 5 Summary

One of the psychologically relevant reasons of the widespread reluctance of working with the dynamics represented by the metric (or, more precisely, with the dynamics controlled by the variations of the set  $\kappa$  of the optional parameters in the metric operator  $\Theta = \Theta(\kappa)$ ) may be seen in the lack of suitable solvable schematic models. This observation may be perceived as one of strong motivations of our present proposal. In the light of Appendix A we may conclude that our manifestly non-Hermitian toy model (7) can really be made compatible with the standard postulates of quantum theory.

We saw that this goal may be achieved in a multitude of ways. Each of them will use a particular multiindex  $\vec{\kappa} \in \mathcal{D}^\Theta$  leading to the reinterpretation of the Hamiltonian which appears manifestly Hermitian in the respective Hilbert space endowed with the *ad hoc* metric  $\Theta \neq I$ .

We have shown that such a strategy leads to a full theoretical consistency of our model. One may find it remarkable that even though our Hamiltonian itself was fixed, the variations of the metric were still changing its observable physical (i.e., quantum and probabilistic) contents. The phenomenological core of our present message may be seen, therefore, in the explicit quantitative illustration of the changes of the horizons of the validity of the model which are caused, at the fixed and unique Hamiltonian, by the mere changes of the parameters in the metric (i.e., by the variations of the selected physical Hilbert space).

In a formal framework our present model appeared unique by its exact solvability involving both the energies and both the left and right eigenvectors. The latter sets form, naturally, a biorthogonal basis which, unexpectedly, just slightly deviates from its more standard Chebyshev-polynomial predecessors. One of the other specific strong merits of the solvability may be seen in the resulting closed-form prescription which defines *all* of the eligible metric operators  $\Theta$  in closed form. In this respect the present model seems to be entirely unique.

In a complementary approach to the construction of the metrics we shifted the emphasis from the universal formulae to the alternative requirement of the sparsity of the metrics. In the light of the sparsity (tridiagonality) of the Hamiltonian we felt encouraged to demand also the existence of the matrices  $\Theta$  which would be sparse and less-parametric. Even in this direction we succeeded. Unfortunately, we were able to indicate, but not able to prove that there might exist further, not yet revealed aspects of the solvability of our present model. Preliminarily, this possibility manifested itself by the piecewise linearity of boundaries of the physical domain  $\Omega \equiv \mathcal{D}^\Theta$  as sampled in Fig. 4 at  $N = 8$ .

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## Appendix A. The operators of metric

It is well known that from the purely mathematical point of view one has an entirely unrestricted freedom of the choice of the concrete representation (say,  $L^2(\mathbb{R})$ ) of the abstract Hilbert space  $\mathcal{H}$  of the admissible states of a quantum system in question.

In the applications of quantum theory this fact often enables us to profit from the simplifications provided by the strict unitary equivalence between various *amended* representations obtained, say, by the Fourier transformation  $L^2(\mathbb{R}) \rightarrow L^2(\mathbb{R})$  which converts the so called coordinate representation (of a single-(quasi)particle system) into the equivalent momentum representation *of the same system*. The formal reason of this equivalence lies in the unitarity of the Fourier mapping.

In the same spirit one may replace  $L^2(\mathbb{R})$  (i.e., the Hilbert space of the quadratically integrable functions  $f(x)$ ) by the slightly more sophisticated Hilbert space  $L^2(\mathbb{R}, \mu)$  in which one merely replaces the usual condition of the quadratic integrability of  $f(x)$  by the more general integration condition using a suitable weight  $\mu(x)$ . The same weighted integration occurs also in the generalized inner product between  $f(x)$  and  $g(x)$  of course,

$$\langle f|g \rangle := \int_{\mathbb{R}} f^*(x)g(x)d\mu(x) \quad \text{in } L^2(\mathbb{R}, \mu). \quad (24)$$

The next step of generalization has been proposed by Scholtz et al [1]. They imagined that in the context of nuclear physics the replacement of the simplest forms of the measure  $d\mu(x)$  by their “smeared” generalizations might simplify some calculations while still leaving the general principles of the

abstract quantum theory unchanged. Thus, for the sufficiently smooth measures  $d\mu(x) = \mu'(x)dx$  this smearing recipe may acquire the comparatively elementary form of the transition to the double integration,

$$\int_{\mathbb{R}} f^*(x)g(x)\mu'(x)dx \longrightarrow \int_{\mathbb{R}} \int_{\mathbb{R}} f^*(x)\Theta(x,y)g(y)dx dy. \quad (25)$$

It defines the inner product in the resulting “smeared” or “sophisticated” Hilbert-space representation  $\mathcal{H}^{(S)}$  via the corresponding smearing operator (usually called “metric” operator)  $\Theta$ .

One of the most transparent and elementary illustrative examples has been constructed by Mostafazadeh [25]. He showed that the special Hilbert space  $\mathcal{H}^{(S)}$  endowed with the *strongly nonlocal* metric of the form

$$\Theta(x,y) \sim \cosh(\omega)\delta(x-y) - \sinh(\omega)\delta(x+y) \quad (26)$$

may be assigned the standard and consistent quantum-mechanical probabilistic interpretation for *every* quantum Hamiltonian  $H$  that can be expressed in terms of the single-particle operators  $\hat{x}^2$ ,  $\hat{x}\hat{p} + \hat{p}\hat{x}$  and  $\hat{p}^2$  (i.e., in particular, for the Hamiltonian  $H_0 = \hat{p}^2$  of a freely moving particle).

In fact, the formal background of our present paper will, incidentally, start from the discrete representation  $\ell^2$  of the Hilbert space rather than from  $L^2(\mathbb{R})$  or  $L^2(\mathbb{R}, \mu)$ . In this sense we merely would have to replace, in this Appendix, the symbols of integrations by summations. At  $N < \infty$  we shall start, in effect, from the “usual” and “friendly” Hilbert space  $\mathcal{H}^{(F)} \equiv \mathbb{R}^N$  of the quantum lattice states<sup>3</sup>. Once one accepts a non-Hermitian matrix  $H \neq H^\dagger$  and declares the latter space “unphysical”, a new, “standard”  $N$ -dimensional Hilbert space  $\mathcal{H}^{(S)}$  (in our present letter, over reals) must be introduced. In such a manner the metric  $\Theta$  becomes an  $N$  by  $N$  Hermitian matrix with positive spectrum while the underlying inner product will read

$$(\vec{a}, \vec{b})^{(S)} = \sum_{\alpha=1}^N \sum_{\beta=1}^N a_\alpha \Theta_{\alpha,\beta} b_\beta. \quad (27)$$

One can immediately notice that such a recipe will convert our present, manifestly non-Hermitian Chebyshevian model (7) into the self-adjoint Hamiltonian.

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<sup>3</sup>with the most common “scalar” inner product of two vectors  $(\vec{a}, \vec{b}) = \sum_{\alpha=1}^N a_\alpha b_\alpha$